

An introduction on bayesian statistics and its applications in cosmology

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In this paper we review the basic concepts on Bayesian statistics for parameter inference and how we can use it in cosmology. This work is organized in such a way that if the reader is only interested in the parameter inference procedure for a model, but not in the cosmological part, he/she can make use of it ignoring only the last part of the paper.

First, we start giving the basic differences between Bayesian and Frequentist statistics. Then we continue with a no so formal introduction on the basic mathematical concepts necessary for a Bayesian parameter inference procedure. Later, we review the most common computational tools at our disposal that can help us to simplify this task. Finally we show how this new concepts can be applied in cosmology.

INTRODUCTION

The beginning of the standard cosmology as it is known today emerges afterwards 1920 when the Shapley-Curtis debate was carried out [?]. This debate was held between the astronomers Harlow Shapley and Heber Curtis, resulting in a revolution for astronomy at that time: “The universe had a larger scale than the Milky Way galaxy”. Several observations at that epoch established the size and the dynamics of the cosmos that could only be explained by Einstein’s General Theory of Relativity. In its infancy, Cosmology was a speculative science that was based only on a few set of data and characterized by a dispute between two cosmological models: the steady state model and the Big Bang (BB) theory. It was not until 1990s when the amount of data was enough to eliminate competitive theories, being awarded the BB model as the most accepted cosmological theory. In that same decade David Schramm herald the “Golden Age of Cosmology” at a National Academy of Sciences colloquium.

Once the new age of cosmological experiments arrived with a very large variety of cosmological data, it was necessary to confront all the cosmological models with those data. The way that it is usually done is using a statistical confrontation. First at all we need to notice that, because we only have one Universe, we can not consider a frequentist interpretation of statistics (we can not create multiple Universes to make a frequentist inference of our models). An alternative interpretation in which we can help us is the Bayesian statistics. On this alternative, probability is interpreted as a degree of belief and it can be useful when no repetitive processes need to be considered.

The principal objective of this work is to give the reader a first step on bayesian parameter inference and how we can use it in cosmology. We consider that the reader is familiarized with the basic concepts of statistics, but not necessarily with Bayesian statistics. Then, we give a not so formal panorama of it, enough to understand the basics concepts of our main objective. This panorama is written in a generic way in such case that, if the reader is not interested in the cosmological section but in the parameter inference one, he/she can draw on the bayesian part.

This paper is organized as follows. We start in section [Bayesian vs frequentist statistic] mentioning the most important differences between the Bayesian statistics and the Frequentist one. Then, in section [A first look on the Bayesian statistics] we present the basic mathematical concepts in Bayesian statistics that are going to be necessary at the moment that we want to estimate a model parameter. Once we have the mathematical concepts, we continue in section [Numerical tools] with the numerical tools at our disposal that can help us to simplify our homework. Such numerical tools are so important given the fact that, in general, it is not possible to apply the mathematical ones analytically when several parameters of our models need to be confronted with data. In section [Bayesian statistics and cosmology] we show how these tools can be used in cosmology, mentioning the different numerical codes free to download on web that are programmed to do this homework and applying them to specific examples. Finally, in section [Conclusions] we conclude this paper.

BAYESIAN VS FREQUENTIST STATISTICS

In this section we introduce the basics to understand the differences about bayesian and frequentist statistics. For an extended review see [?], [?], [?], [?] or/and [?].

Fundamentally, the main difference between bayesian and frequentist is its definition of probability. In frequentist statistic probability has mining in a limiting case of repeating measurements

$$P = \frac{n}{N} \quad (1)$$

where n denotes the number of successes and N the total number of trials. Frequentist define probability as the limit for the number of independent trials going to infinity. Then, **for frequentist, probabilities are fundamentally related to frequencies of events**. On the other hand in bayesian statistic the concept of probability is extended to cover degrees of certainty about statement. **For Bayesians, probabilities are fundamentally related to our own knowledge about an event**.

If we consider that x is a random variable related with a particular event and $P(x)$ its corresponding probability distribution, for both cases the same rules of probabilities apply, which are¹

$$P(x) \geq 0 \quad (2a)$$

¹ This rules are defined for a continuous variable. However, the corresponding discreet definition can be given immediately by replacing $\int \rightarrow \sum$.

$$\int_{-\infty}^{\infty} dx P(x) = 1 \quad (2b)$$

For mutually exclusive events

$$P(x_1 \cup x_2) = P(x_1) + P(x_2) \quad (2c)$$

In general

$$P(x_1, x_2) = P(x_1)P(x_1|x_2) \quad (2d)$$

In words, the last rule can be explain as: the probability of x_1 and x_2 to happen is the probability of x_1 times the conditional probability of x_2 given that x_1 has already happened.

Frequentist statistics

Any frequentist inferential procedure relies on three basic ingredients: the data, a model and an estimator procedure. The central assumption in frequentism is that the data has a definite but unknown, underlying distribution to which all inference pertains.

The *data* is a measurement or observation which we denote by X , taking values in a corresponding sample space. Then, a *sample space* of an observation X can be defined as a measurable space (x, \hat{B}) containing all values that X can take upon measurement.

In frequentist statistics it is considered that there is a probability function $P_0 : \hat{B} \rightarrow [0, 1]$ on the sample space x representing the “ true distribution of the data”

$$X \sim P_0$$

The second ingredient mentioned above is the model. For frequentist statistics a model Q is a collection of probability measures $P : \hat{B} \rightarrow [0, 1]$ on the sample space (x, \hat{B}) . The distributions P_θ are called model distributions. In this approach θ is unchanged. Of course $P_\theta(x)$ have to follow the rules mentioned at the beginning of this section.

A model Q is said to be well-specified if it contains the true distribution of the data P_0 , i.e.

$$P_0 \in Q$$

Finally we need a point-estimator(or estimator) for P_0 . An estimator for P_0 is a map $\hat{P} : x \rightarrow Q$, representing our “best guess” $\hat{P} \in Q$ for P_0 based on the data X .

Hence, the frequentist statistic is based in trying to respond the following questions: “what does the data make clear about P_0 ?”, “from the data, what can we say about the mean of P_0 ?”, etcetera.

Bayesian statistics

As is explained in [?] in bayesian statistics, data and model form two factors of the same space, i.e. no formal distinction is made between measured quantities X and parameters θ . One may envisage the process of generating a measurement outcome $Y = y$ as two draws, one draw for Θ (or Q) to select a value of θ (or distribution P_θ) and a subsequent draw for P_θ to arrive at $X = x$. This perspective may seem rather absurd in view of the definitions made in the subsection above. In this way an element P_θ of the model is interpreted simply as the distribution of X given the parameter value θ , i.e. as the conditional distribution $X|\theta$.

A little more clear

It is so important to understand the differences between both kind of approximations. For it, let us review with an example in this subsection the basic differences about the frequentist and bayesian statistics.

In table ?? we have a very little review of the most important differences about the two approximations. In the other side in the next example we present an experiment seen in both points of view. Because we are interested in

Frequentist	Bayesian
Data are a repeatable random sample. There is a frequency	Data are observed from the realized sample
Underlying parameters remain constant during this repeatable process	Parameters are unknown and described probabilistically
Parameters are fixed	Data are fixed

TABLE I: Main differences between the bayesian and frequentist interpretations.

knowing both descriptions we show only the basic results of the procedures and we analyze the results in the point of view of the frequentist and bayesian statistics.

Example.- In this experiment you have a coin that has a probability p that when is through, it is head and a probability $1 - p$ to be tail. Then, trying to estimate p you flip the coin 14 times (spoiler alert: $p=0.5$). The result is head 10 times. Now, what we are interested about is in the next two possible events. To be precise: “What is the probability that in the next two tosses we will get two heads in a row?”

- *Frequentist approximation.* As we mentioned before in frequentist statistics probability is related with a frequency of events. In this way we have that our best estimate for p is $P(head) = \text{No.heads}/\text{No.total} = 10/14$. So, the probability to have 2 heads in a row is $P(2heads) = P(head)P(head) \simeq 0.51$.
- *Bayesian approximation.* Now in the bayesian approach p is not a value, it is a random variable with its own distribution. The distribution must be defined by the existing evidence. In this example a good distribution for p is a binomial distribution. Then, by considering a uniform distribution as our prior information (we do not know anything about p) we have that the probability of having two heads is

$$P(2heads|D) = \frac{B(13, 5)}{B(11, 5)} = 0.485$$

where $B(x, y)$ is the beta function. This distribution appears given the fact that $B(1, 1)$ is the uniform distribution which we consider as our prior.

We can see that both approximations arrive at different results. In one of them, since we consider probability as a frequency of events we have a bigger probability to have two heads in a row than when we consider probability as our knowledge about the experiment. However, in both cases the probability defers from the real one ($P(2heads) = 0.25$) because we have not enough data for our estimations.

Note: If you are not familiarized with bayesian statistics, please be not scared of this last example. In the next section we will introduce the basic concepts to understand the bayesian part of it and then we will go back to this example and we will solve it using the new tools learned.

A FIRST LOOK OF THE BAYESIAN STATISTICS

Before to start with the applications of bayesian statistics in cosmology it is necessary to know the most important tools for the bayesian procedure. In this section we review them in an informal way, keeping in mind that more formal readers can look for the formal treatment in the literature.

Bayes theorem, prior and posterior distributions

When a statistician is interested in working in the Bayes framework there are 3 concepts that are necessary to understand before to interpret whatever result that he could obtain: the Bayes theorem, priors and posterior distributions. In this section we quickly review these concepts and then we take back the example about the coins given in the last section in order to exemplify them.

The Bayes theorem. The Bayes theorem is a direct consequence of the axioms of probability (??). We can see that from (??) without loss of generality we can rewrite $P(x_2, x_1) = P(x_2)P(x_2|x_1)$. But, of course, one expect that the

relation $P(x_1, x_2) = P(x_2, x_1)$ have to be fulfill. With this we arrive at the Bayes formula

$$P(x_2|x_1) = \frac{P(x_2)P(x_1|x_2)}{P(x_1)} \quad (3)$$

As we mentioned before, in the Bayes framework, data and model are part of the same space. In this way considering $x_1 \rightarrow D$ as a set of data, and $x_2 \rightarrow H$ as our "hypothesis" we can rewrite the above equation in the Bayesian statistics without lost of generality as

$$P(\theta, H|D) = \frac{P(\theta, H)P(D|\theta, H)}{P(D)} \quad (4)$$

Here we have added the extra term θ in order to specify that our hypothesis can depend on several parameters. The above equation is the so-called *Bayes theorem* and it is the principal tool in a Bayesian inference procedure. In this result $P(\theta, H|D)$ is called the *posterior* probability for the model. $L(D; \theta) \equiv P(D|\theta, H)$ is called the *Likelihood* and we will concentrate on it in a future section. $P(D|\theta, H)$ is called the *prior*, and expresses what we know about our model before to know the data. This prior can be fixed depending on previous experiment results or the theory that we are working with. $P(D)$ is the evidence of our model. We can notice that this evidence acts only as a normalization factor

$$P(D) = \int d\theta P(D|\theta, H)P(\theta, H). \quad (5)$$

Then, this quantity is usually ignored for practical proposes when the parameter space of a unique model is tested. In the other side if what we are interested about is in a comparative between 2 or more models, the evidence plays an important role when we choose which model is more likely, whatever the parameters are. For the propose of this work we are not interested in this scenario and we will ignore it every time.

We can notice here that we have added a new ingredient in our Bayes description, which is the hypothesis. An hypothesis is our best guess of the model that best matches with the data, $H = Q_{best}$.

We can see that Bayes theorem has an enormous implication respect to an statistical inferential point of view. In a typical scenario we can collect some data and wish to interpret them in terms of a model. However, what we can usually do it is the opposite, is, we have first a set of data and then we can confront a model considering what is the probability that our model matches with the data. As we can see from (??) Bayes theorem gives us a tool where we can relate both scenarios. Then, thanks to the Bayes theorem, in principle, we can know what is the "real" model that best fixes the data.

Example.- We consider again the example shown in the last section. What we are interested in is knowing what is the probability $P(2heads|D)$ (D = our 14 data) to have 2 heads in a row given the 14 data that we already have. For simplicity we do not update p between the two tosses and we assume that both tries are independent. To obtain the result that we expect we need to calculate

$$P(2heads|D) = \int_0^1 P(2heads|p)P(p|D)dp \quad (6)$$

where $P(p|D)$ is the probability of the data given our model p and $P(2heads|p)$ is the probability of our model p given that we had 2 heads.

Because we are considering that both tries are independent we have

$$P(2heads|p) = [P(head|p)]^2 \quad (7)$$

where $P(head|p)$ is the probability of our model p given that we obtained a head. A good model for our experiment given the data is a binomial distribution

$$P(D|p) = \binom{14}{10} p^{10} (1-p)^4 \quad (8)$$

Then

$$P(head|p) = p \Rightarrow P(2head|p) = p^2 \quad (9)$$

Now we need to compute $P(p|D)$. Using the bayes theorem we have

$$P(p|D) = \frac{P(D|p)P(p)}{P(D)} \quad (10)$$

A very convenient prior distribution for this scenario is the *beta distribution* $Beta(p; a, b)$ defined as

$$Beta(p; a, b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} p^{a-1} (1-p)^{b-1} \quad (11)$$

where Γ is the gamma function. So

$$P(p) = Beta(p; a, b) \quad (12)$$

We are interested in the explicit form of $P(p|D)$ in such case we need to compute $P(D)$. Introducing (??) and (??) into (??) we have

$$P(D) = B(10+a, 4+b) \equiv \frac{\Gamma(10+a)\Gamma(4+b)}{\Gamma((10+a)+(4+b))} \quad (13)$$

and then

$$P(p|D) = \frac{p^{10+a-1}(1-p)^{4+b-1}}{B(10+a, 4+b)} \quad (14)$$

Now what we need to know are the values of a and b . If we assume that we do not know anything about p we can consider our prior as a normal distribution which corresponds to take $a = b = 1$. Notice from figure ?? that our posterior result (??) does not agree with the real result that we know ($p=0.5$). What we would like to expect is that our posterior distribution is centered at $p = 0.5$ with a very thin distribution. Of course, this disagreement could be fixed if we continue increasing our experimental results.

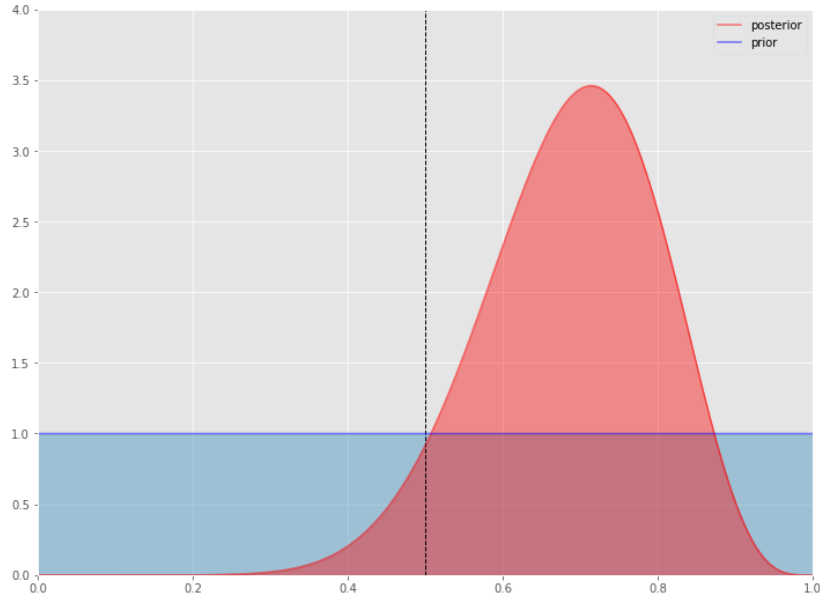


FIG. 1: Prior and posterior distribution in the coin example. The black line corresponds with the well known real value of p . Solving the integral in (??) with (??) and (??) we arrive at the final result obtained in the above section

$$P(2heads|D) = \frac{B(13, 5)}{B(11, 5)} = 0.485 \quad (15)$$

Updating the probability distribution for a model

As we saw in the coin example, due to the fact that we have not enough data we did not arrive to the real value of p . If we would like to be closer to the real one we should continue flipping the coin until the amount of data were enough. If we continue with the coin example and, we say, after throwing 100 times the coin we obtain 56 heads, and then after throwing 500 times the coin we obtain 246 heads, we should obtain a more tiny distribution centered near $p = 0.5$ (see fig. ??). In this way, it is clear that in order to confront a parameter model and be more accurate of the most probable (“real”) value of it, it is necessary to increase the amount of data (and the capacity for precision) in any experimentation. Then, what we have here is that we will have some model’s parameters that has to be confronted with different set of data. There are two ways we can do this: first is regarding the sum of all the sets of data that we have, or consider each data set as the new data, but our prior information has to be set by what we know about the previous set of data. What is important in bayes statistic is that it doesn’t matter wich of the 2 possibilities we choose. In the coin context it means that it is equivalent to start with the prior given in figure ??-a and considering the 500 data we can arrive at the posterior ??-d or start with ??-c as our prior and consider the last 400 data to obtain the same posterior ??-d.

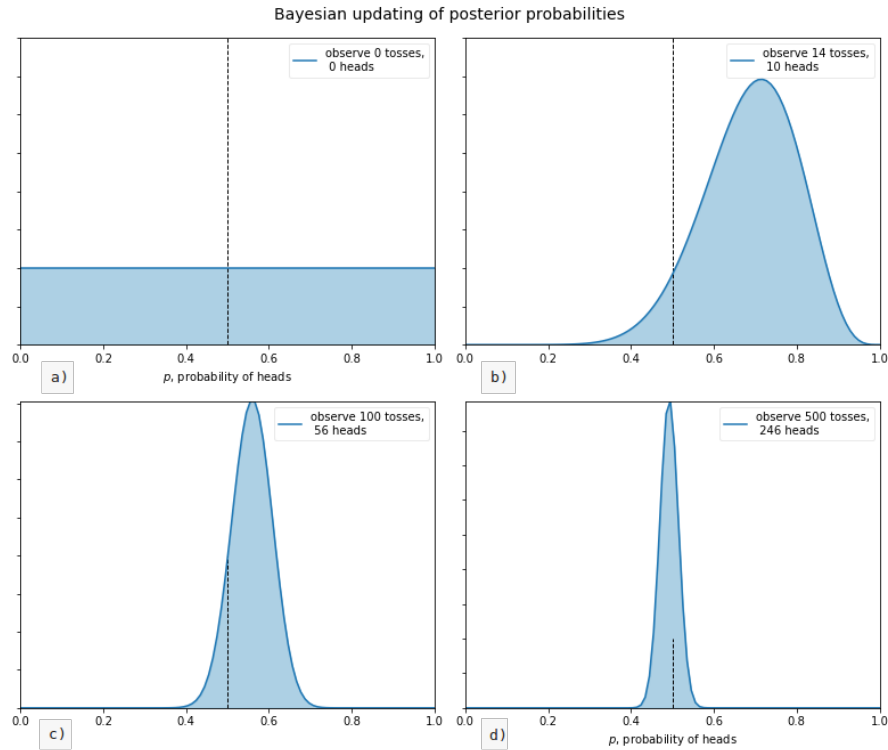


FIG. 2: Posterior distributions of p when our data is increased. Notice that while we continue increasing the experimental results, the posterior distribution starts to be more localized near the real value $p = 0.5$.

In fact, if we rewrite Bayes theorem putting explicitly that all probabilities are conditional of some prior information I

$$P(\theta, H|DI) = \frac{P(\theta, H|I)P(D|\theta, HI)}{P(D|I)} \quad (16)$$

and then we consider a new set of data D' , letting the old data become part of the prior information $I' = DI$ we arrive at [?]

$$P(\theta, H|DI') = \frac{P(\theta, H|I)P(DD'|\theta, HI)}{P(DD'|I)} = P(\theta, H|[DD']I) \quad (17)$$

where we can see explicitly the equivalence of the 2 different options for analyzing our results.

About the Likelihood

As we mentioned before the evidence in the Bayes theorem is not usually important when we try to do any inference procedure in the parameter space of a model. Then, we can fix it as $P(D) = 1$ without loss of generality. In this way, if we ignore the prior² we can identify the likelihood with $P(H|D)$ and thus by maximizing it we can find the most likely model (or model's parameters) given the data. However having ignored $P(D)$ and the prior this approach cannot give in general a goodness of fit and thus cannot give an absolute probability for a given model. However it can give relative probabilities. In the other side, it is possible to report results independently of the prior by using the *Likelihood ratio*. The likelihood at a particular point in parameter space can be compared with the one that best fit the observations, L_{max} . Then we can say that a model is acceptable if the likelihood ratio

$$\Lambda = -2 \ln \left[\frac{L(D; \theta, H)}{L_{max}} \right] \quad (18)$$

is bigger than a given value.

Let us assume we have a posterior distribution, which is single-picked. We consider that $\hat{\theta}$ corresponds with the peak of the distribution (most probable) or the mean

$$\hat{\theta} = \int d\theta \theta P(\theta, H|D). \quad (19)$$

We consider that our model is well-specified and that the expectation value of $\hat{\theta}$ corresponds with the real value θ_0

$$\langle \hat{\theta} \rangle = \theta_0, \quad (20)$$

then we say that $\hat{\theta}$ is *unbiased*. Considering a Taylor expansion of the log likelihood

$$\ln L(D; H) = \ln L(D; H_0) + \frac{1}{2}(\theta_\alpha - \theta_{0\alpha}) \frac{\partial^2 \ln L}{\partial \theta_\alpha \partial \theta_\beta} (\theta_\beta - \theta_{0\beta}) + \dots \quad (21)$$

where H_0 corresponds with the real model (and/or parameter of the model). In this way we have that the likelihood can be expressed as a multi-variable likelihood given by

$$L(D; H) = L(D; H_0) \exp \left[-\frac{1}{2}(\theta_\alpha - \theta_{0\alpha}) H_{\alpha\beta} (\theta_\beta - \theta_{0\beta}) \right] \quad (22)$$

where

$$H_{\alpha\beta} = \frac{\partial^2 \ln L}{\partial \theta_\alpha \partial \theta_\beta} \quad (23)$$

is called the *Hessian matrix* and it controls whether the estimates of θ_α and θ_β are correlated or not. If it is diagonal, the estimates are uncorrelated.

The above expression for the likelihood is a good approximation always that our posterior distribution possess a single-pick. However in a general way the likelihood may not be well described by a gaussian expression at levels with set the interesting credibility levels. It is worth mentioned that if the data error are Gaussianly distributed, then the likelihood for the data will be a Gaussian function, as well. In fact, this is always true if the model depends linearly on the parameters [?]. In the other side, if the data are not Gaussianly distributed we can resort to the central limit theorem. In this way the central limit theorem will tell us that the resulting distribution will be better approximated by a multi-variate Gaussian [?].

Justifying the neglect of the priors

In this section we are interested in justifying the neglect of the prior in the Bayes theorem. For this, we follow the example given in [?]. In this example there are 2 people A and B that are interested on the measurement of a

² It is expected that the real value of a given parameter is independent of the election of the prior.

given physical quantity θ . A and B have different prior beliefs regarding the possible value of θ . This discrepancy could be given by the experience, such as the possibility that A and B have made the same measurement in another moment being alone. Let us denote their priors by $P(\theta|I_i)$ ($i = A, B$) and let us assume that they are described by two Gaussian distributions on mean μ_i and variance Σ_i^2 . Now, A and B make a measurement together and they obtain the value $\theta_0 = m_1$. If we consider that the experiment is such as that our parameters are uncorrelated we can rewrite (??) as

$$L(D; HI) = L_0 \exp \left[-\frac{1}{2} \frac{(\theta - m_1)^2}{\sigma^2} \right] \quad (24)$$

Replacing the hypothesis H by the continuous variable θ the Bayes theorem for the model of A and B is

$$P(\theta|m_1) = \frac{L(m_1; \theta I_i) P(\theta|I_i)}{P(m_1|I_i)} \quad (25)$$

where we have used the notation given in (??). Then the posterior of A and B are again Gaussian with means

$$\hat{\mu}_i = \frac{m_1 + (\sigma/\Sigma_i)^2 \mu_i}{1 + (\sigma/\Sigma_i)^2} \quad (26)$$

and variance

$$\tau_i^2 = \frac{\sigma^2}{1 + (\sigma/\Sigma_i)^2}, \quad (i = A, B) \quad (27)$$

Thus if the likelihood is more informative than the prior i.e. $(\sigma/\Sigma) \ll 1$ the posterior means of A and B will converge towards the measured value, m_1 . As more and more data are obtained one can simply replace the value of m_1 in the above equation by the mean $\langle m \rangle$ and σ^2 by σ^2/N . Then, we can see that the initial prior μ_i of A and B will progressively be overridden by the data. This process is illustrated in figure ??

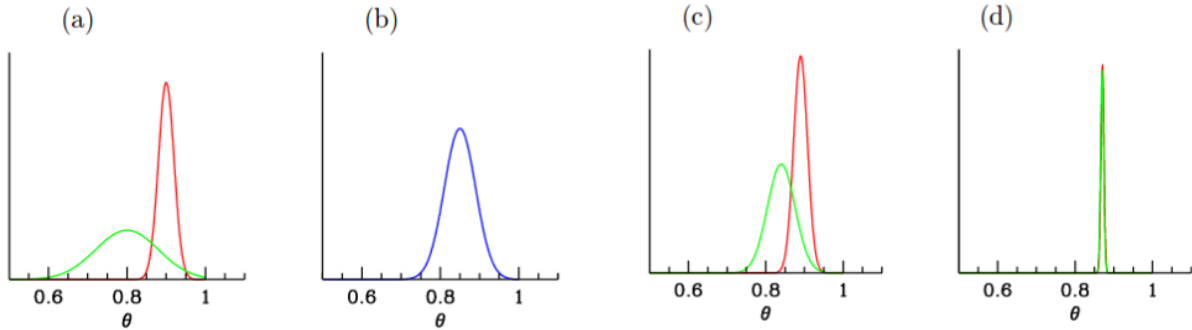


FIG. 3: Converging views in Bayes inference, taken from [?]. A and B have different priors $P(\theta|I_i)$ about a value of θ (panel (a)). Then, they observe one datum with likelihood $L(\theta; HI)$ (panel (b)), after which their posteriors $P(\theta|m_1)$ (panel (c)) represents their updates. Then, after observing 100 data it can be seen how both posteriors are practically indistinguishable (panel (d))

Chisquare and goodness of fit

We mentioned that it is necessary to maximize the likelihood in order to obtain the more likely model (or model parameters) given the data. If we consider the Gaussian approximation given in (??) we can see that the likelihood will be maximum always that the quantity

$$\chi^2 \equiv (\theta_\alpha - \theta_{0\alpha}) H_{\alpha\beta} (\theta_\beta - \theta_{0\beta}) \quad (28)$$

is minimum. The quantity χ^2 is usually called *chisquare* and is related with the Gaussian likelihood via $L = L_0 e^{-\chi^2/2}$. In this way we can say that the maximizing of a Gaussian likelihood procedure and the minimizing of a chisquare procedure are equivalent. However, as we mentioned before, there are some circumstances where the likelihood can not be well specified by a Gaussian distribution, then, in that cases the chisquare and the likelihood are not longer equivalent.

We can consider a probability distribution for different values of χ^2 around its minimum. This is the χ^2 distribution for $v = n - M$ degrees of freedom where n is the number of independent data points and M the number of parameters. In this way we can calculate the probability that an observed χ^2 exceeds by chance a value $\hat{\chi}$ for the correct model. This probability is given by [?] $Q(v, \hat{\chi}) = 1 - \Gamma(v/2, \hat{\chi}/2)$ where Γ is the incomplete Gamma function. Then, the probability that the observed χ^2 (even the correct model) is less than a given value $\hat{\chi}^2$ is $1 - Q$. This statement is strictly true if errors are Gaussian and the model is a linear function of the likelihood, i.e., for Gaussian likelihoods.

If we evaluate the quantity Q in the best fit of the chisquare (i.e. its minimum) we can have a measure of the goodness of the fit. If Q is small (small probability) we can interpret it as:

- The model is wrong and can be rejected
- The errors are underestimated
- The measurement errors are not Gaussianly distributed.

In the other side if Q is too large there are some reasons that could cause such overestimation:

- Errors have been overestimated
- Data are correlated or non-independent
- The distribution is non-Gaussian.

Contour plots and confidence regions

Once the best fit parameters are obtained we would like to know if there are confidence regions where other parameters could be considered as a good candidate for our model. The most logical election is to consider parameters inside a compact region around the best fit value. Then, a natural choice is to consider regions with a constant χ^2 boundaries. In the case that χ^2 possesses more than 1 minimum it is said that we have more than one non-connected confidence region. For multi-variate Gaussian distributions (as the likelihood approximation (??)) these are ellipsoidal regions. In this section we exemplify how to calculate the confidence regions following [?].

We can consider a little perturbation from the best fit of chisquare $\Delta\chi^2 = \chi^2 - \chi_{best}^2$. Then we can use the properties of χ^2 distribution to define confidence regions for variations on χ^2 to its minimum. In Table ?? we can see the typical 68.3%, 95.4% and 99.5% confidence levels as a function of number of parameters for the joint confidence level. In the case of Gaussian distribution (as the likelihood) these correspond to the conventional 1, 2 and 3 σ .

σ	p	$M = 1$	$M = 2$	$M = 3$
1σ	68.3%	1.00	2.30	3.53
2σ	95.4%	4.00	6.17	8.02
3σ	99.73%	9.00	11.8	14.20

TABLE II: $\Delta\chi^2$ for the conventional 68.3%, 95.4% and 99.73% as a function of the number of parameters for the joint confidence level.

The general cooking recipe to compute constant- χ^2 confidence regions are as follows: After having found the best fit by minimizing χ^2 (or maximizing the likelihood) and if Q for the best parameters is acceptable, then:

1. Let M be the number of parameters, n the number of data and p be the confidence limit desired.
2. Solve the equation:

$$Q(n - M, \min(\chi^2) + \Delta\chi^2) = p \quad (29)$$

3. Find the parameter region where $\chi^2 \leq \min(\chi^2) + \Delta\chi^2$. This defines the confidence region.

Marginalization

It is clear that a model can (in general) depend on more than one parameter. However, most of these parameters θ_i may be uninteresting. For example, these parameters can correspond with nuisance parameters like calibration factors or it may be that we are interested in constraints on only one parameter at the time rather than on the joint constraints on 2 or more parameters simultaneously. Then we marginalize over the uninteresting parameters by

$$P(\theta_1, \dots, \theta_j, H|D) = \int d\theta_{j+1} \dots d\theta_m P(\theta, H|D) \quad (30)$$

where m is the total number of parameters in our model and $\theta_1, \dots, \theta_j$ denote the parameters that we are interested in.

Fisher Matrix

Once we have a set of data it is important to know how accurate we can estimate model parameters. Fisher [?] proposed a way to solve this issue 70 years ago. In this section we review the main results of his work following the procedure given in [?].

First at all we consider again the gaussian likelihood. As we can notice the Hessian matrix $H_{\alpha\beta}$ enclose information of the parameters errors and their covariance. More specifically when all parameters are fixed except one (e.g. the i th parameter) the error on that parameter is $1/\sqrt{H_{ii}}$. These errors are called conditional errors, although they are not usually used.

A quantity that arises naturally with gaussian likelihoods to forecast the precision of a model is the so-called *Fisher information matrix*

$$F_{ij} = - \left\langle \frac{\partial^2 \mathcal{L}}{\partial \theta_\alpha \partial \theta_\beta} \right\rangle \quad (31)$$

where

$$\mathcal{L} = \ln L \quad (32)$$

It is clear that $F = \langle H \rangle$. Here average is over observational data.

As we can see from eq. (??) when we have independent data sets, the complete likelihood is the product of the likelihoods and then the fisher matrix for independent data sets is the sum of the individual fisher matrices.

A pedagogical and the easiest case is working in the one-parameter case θ_i and considering a gaussian likelihood. In this scenario we have that

$$\Delta \mathcal{L} = \frac{1}{2} F_{ii} (\theta_i - \theta_{0i})^2 \quad (33)$$

when $2\Delta \mathcal{L} = 1$ and by identifying it with the $\Delta \chi^2$ corresponding to 68% confidence level, we notice that $1/\sqrt{F_{ii}}$ yields the $1 - \sigma$ displacement for θ_i . In the general case

$$\sigma_{ij}^2 \geq (F^{-1})_{ij} \quad (34)$$

Thus when all parameters are estimated simultaneously from the data the marginalized error is

$$\sigma_{\theta_i} \geq (F^{-1})_{ii}^{1/2} \quad (35)$$

The beauty of the Fisher matrix approach is that there is a simple prescription for setting up the Fisher matrix knowing only your model and your measurement uncertainties and that under the assumption of a gaussian likelihood, the Fisher matrix is the inverse of the covariance matrix. So all you have to do is set up the Fisher matrix and then invert it to obtain the covariance matrix (that is, the uncertainties on your model parameters). In addition if it can be computed quickly, it also enables one to explore different experimental set ups and optimize the experiment.

The whole point of the Fisher matrix formalism is to predict how well the experiment will be able to constrain the model parameters, before doing the experiment and in fact without even simulating the experiment in any detail. We can then forecast the results of different experiments and look at trade offs such as precision versus cost. In other words, we can engage in experimental design.

The \leq in (??) is called the Kramer-Rao inequality. We can see that the Fisher information matrix represent a lower bound for the errors. Only when the likelihood is gaussianly distributed the \leq is transformed in $=$. However as we saw in [About the likelihood] a gaussian likelihood is only applicable to some circumstances, being generally impossible to be applied. So the key is to have a good understanding of our theoretical model in such a way that we can construct a gaussian likelihood.

NUMERICAL TOOLS

In a typical scenario it is not possible to compute the posterior analytically in our Bayesian inference procedure. In this way it is important to know, once we have all the necessary mathematical tools to make a bayesian estimation, all the numerical tools at our disposal that can help us in our parameter estimation. Of course we could have several numerical candidates that could help us in this homework, but in this section we present only the typical one (and the easier) used in cosmology: the Monte Carlo Markov Chain (MCMC) with the Metropolis Hasting algorithm (MHA). Additionally in this section we present some useful details that we have to take into account if we want to make efficient our computation.

Important: In the next section we are going to apply, using a python code, all this new techniques to a cosmological example. The code is very simple and is programed using the PyMC module of Python. You can see it in appendix [B]. We present this code in order to make easier the homework for the reader that is starting with the parameter inference techniques and is interested in programing his/her own MCMC code. Notice that if you are not interested in a cosmological model, it is enough to change it in the function "model" by the one that you must prefer.

MCMC techniques for parameter inference

The purpose of a MCMC algorithm is to construct a sequence of points in a parameter space (called "chain") in order to evaluate the posterior of eq. (??) for the usual case where analytical solutions do not exist or are insufficiently accurate. In this section we review the basics results for this procedure in a simplistic way but for curious readers it is recommendable to see [?], [?], [?] or only for markov chains [?].

A sequence X_1, X_2, \dots of random elements of some set is a *Markov chain* if the conditional distribution of X_{n+1} given X_1, \dots, X_n depends on X_n only. In other words a Markov chain is a process where we can do predictions of the future based only in the information given at the present. An important property of a Markov chain is that they can be shown to converge to a stationary state were successive elements of the chain are samples from the target distribution, in our case the posterior $P(\theta, H|D)$. In this way we can estimate all the usual quantities of interest from it (mean, variance, etc). The number of points required to get good estimates is said to scale linearly with the number of parameters, so very quickly become much faster than grids as the dimensionality increases.

The target density is approximated by a set of delta function

$$p(\theta, H|D) \simeq \frac{1}{N} \sum_{i=1}^N \delta(\theta - \theta_i) \quad (36)$$

In this procedure the posterior mean is given by

$$\langle \theta \rangle = \int d\theta \theta P(\theta, H|D) \simeq \frac{1}{N} \sum_{i=1}^N \theta_i \quad (37)$$

where \simeq follows because the sample θ_i are generated from the posterior by construction. Then, we can estimate any integrals (such as the mean, variance, etc) as

$$\langle f(\theta) \rangle \simeq \frac{1}{N} \sum_{i=1}^N f(\theta_i) \quad (38)$$

As was mentioned, in a Markov chain it is necessary to generate a new point θ_{i+1} in our chain from the present point θ_i . However, we would like to accept this point as a new point in the chain with a probability which depends on the ratio of the new and old target densities. The distribution of steps is called the *proposal distribution*. In this way what we need now is an algorithm which can help us to accept/refuse the new points. The most popular algorithm is the so-called Metropolis Hasting algorithm and in what follows we explain in what it consists.

Metropolis Hasting algorithm

The *Metropolis Hasting algorithm* (MHA) [?] is the simplest MCMC algorithm. For it, starting from a random initial point θ_0 , with associated posterior probability $p_0 = p(\theta_0, H|D)$, we need to propose a candidate θ_c by drawing from the *proposal distribution* $q(\theta_0, \theta_c)$. Then, the probability of acceptance of a new point is given by

$$p(\text{acceptance}) = \min \left[1, \frac{p_c q(\theta_c, \theta_0)}{p_0 q(\theta_0, \theta_c)} \right] \quad (39)$$

If the proposal distribution is symmetric, the algorithm is reduced to the *Metropolis algorithm*

$$p(\text{acceptance}) = \min \left[1, \frac{p_c}{p_0} \right] \quad (40)$$

In this way the complete algorithm can be expressed following this steps:

1. Choose a random initial condition θ_0 in parameter space and compute the posterior distribution
2. Generate a new candidate from a proposal distribution in the parameter space and compute the corresponding posterior distribution
3. Accept (or not) the new point with the help of the Metropolis Hasting algorithm
4. If the point is not accepted, repeat the previous point in the chain
5. Repeat step 2-4 until you have a chain large enough

A first example in parameter inference using a MCMC technique with a MHA

In order to exemplify the numerical tools learned in this section, let us go back to the example of the coins seen in subsection [Bayes theorem, prior and posterior distributions]. Because we are interested that the reader understands what is the basic procedure given in this section, let us only try to estimate what is the value of p (or region of values for p) that best matches our data (the 14 times that the coin was trough). For it we calculate the posterior distribution (??) using the MHA.

As before we consider a Likelihood given by a binomial distribution (??) and a normal distributed prior (??) ($a = b = 1$). As our first “guest” for p we take $p_0 = 0.1$. We generate a new candidate p_c as $p_c = p_i + G(p_i, \sigma)$, where $G(p_i, \sigma)$ is our Gaussian proposal distribution centered at p_i and with variance $\sigma = 0.02$; p_i is the current value of p that for our first step is $p_i = p_0$. Then, we compute the Metropolis Hasting algorithm in a Python code as can be seen in appendix [A]. Our final result, fig. ??, was a posterior distribution that matches very well with the posterior that was calculated analytically. Notice that we have plotted our 95% confidence regions (black line).

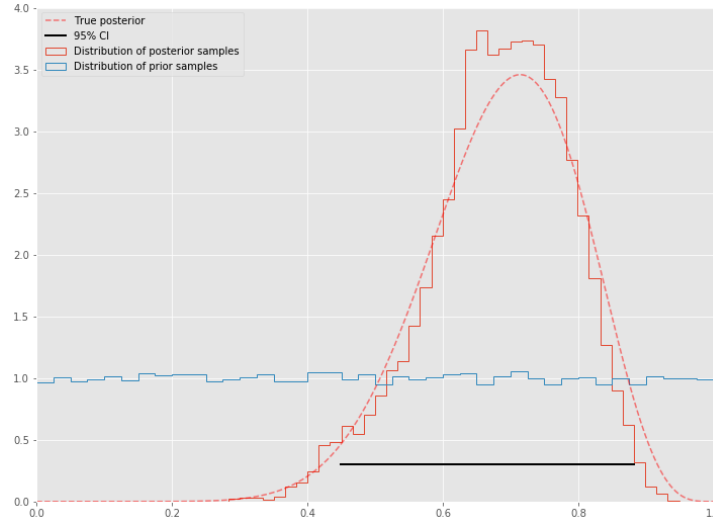


FIG. 4: Posterior distribution for our example. We plot the prior distribution (blue), true posterior (dashed-red) and the posterior calculated by the MHA (red). We plot 95% confidence region for the estimation of p .

To complete the example we show in figure ?? the Markov Chain generated by our code. We can notice that the chain oscillates around a middle value. This behavior is expected due to the fact that we have not enough data to constrain more accurately the value of p and then there are several values for p that can matches with enough precision our data.

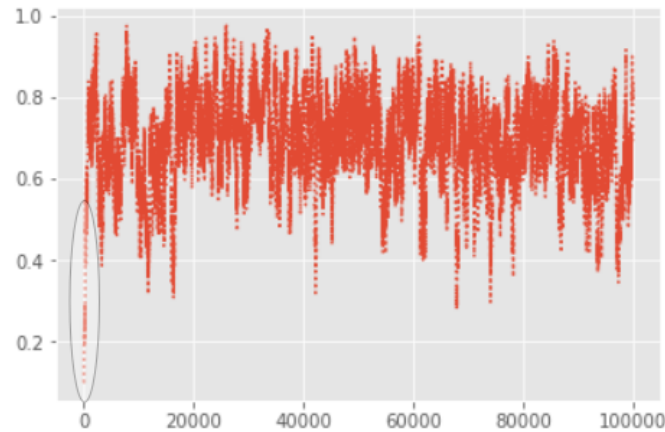


FIG. 5: Markov chain. We use $p_0 = 0.1$ as our first “guest” for p .

Note: In appendix [A] we computed our MCMC algorithm using an explicit code of the MCMC process. However, in Python there are some modules that can help us to simplify our life. For example PyMC is a Python module that implements statistical models and fitting algorithms, including the MCMC algorithm. It is convenient to learn how to use this module if you are interested in construct your own algorithm to constrain a(some) parameter(s).

Some useful details

About the proposal distribution. The choice of a proposal distribution q is crucial for the efficient exploration of the posterior. If the scale of q is too small compared with the scale of the target in the sense that the typical jump is small, then the chain may take a very long time to explore the target distribution which imply that the algorithm will be very inefficient. In the other side, if the scale of q is too large, the chain gets stuck and it does not jump very frequently. In our example we used a Gaussian distribution with a variance (step) $\sigma = 0.02$. This value was taken because we explored, by hand, different values for σ and we took the one that looked to approx more quickly to the real main value of p .

In order to fix this issue in a more efficient way, it is recommendable to run an exploratory MCMC, compute the covariance matrix from the samples, and then re-run with this covariant matrix as the covariance of a multivariate Gaussian proposal distribution. Of course, this process can be computed a couple of times before to run the “real” MCMC.

About the burn-in. It is important to notice that when we start a chain we will have a region of points outside the stationary region where the chain converge (In our chain we could consider those points as the ones inside the ellipse in figure ??). This early part of the chain (called “burn-in”) must be ignored and then the dependence on the starting point must be lost. For it, it is important to have a convergence test which can help us to know when the chain has converged.

Convergence test. It is clear that we need a test to know when our chain has converged. However we need to be warned that the point in our chain is not in a “false convergent point” or a locally maximum point. In this way we need that our rule takes into account this possible difficulty. The simplest way (the informal way) to know if our chain is converging is running several chains starting with different proposal initial point for the parameter that we are interested about to estimate. Then, if we see, by eye, that all the chains looks to converge to a single region of the possible value for our parameter, we could consider that our chains are converging to that region.

Taking again the experiment of the coins, we can run several chains for the above example and try to estimate if the value (the region) of p that we found is an sttionary value (region). In figure ?? we plotted 5 different Markov

chains with initial “guest” condition $p = 0.2, 0.3, 0.5, 0.7, 0.9$. As we expected from the analytical result, all the chains looks to concentrate near the same value.

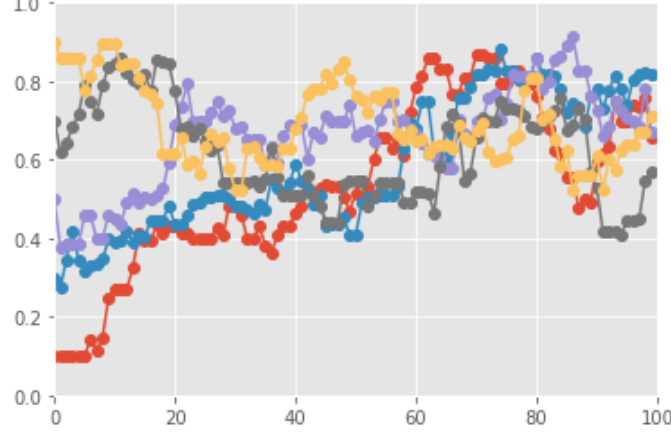


FIG. 6: Multiple MCMC. We calculate 5 Markov chains to estimate convergence of our chains.

The above convergence method explained is very informal and we would like to have a better way to ensure that our result is correct. The classical test used for it is the *Gelman-Rubin* (1992) convergence criterion. This is (following [?], [?]) by starting M chains with very different initial point and N points per chain. Then if θ_i^j is a point in parameter space of position i and chain j , we need to compute the mean of each chain

$$\langle \theta^j \rangle = \frac{1}{N} \sum_{i=1}^N \theta_i^j \quad (41)$$

and the mean of all the chains

$$\langle \theta \rangle = \frac{1}{NM} \sum_{i=1}^N \sum_{j=1}^M \theta_i^j. \quad (42)$$

Then the chain-to-chain variance B is

$$B = \frac{1}{M-1} \sum_{j=1}^M (\langle \theta^j \rangle - \langle \theta \rangle)^2 \quad (43)$$

and the average variance of each chain is

$$W = \frac{1}{M(N-1)} \sum_{i=1}^N \sum_{j=1}^M (\theta_i^j - \langle \theta^j \rangle)^2 \quad (44)$$

If our chains converge, W and B/N must agree. In fact we say that the chain converges when the quantity

$$\hat{R} = \frac{\frac{N-1}{N}W + B(1 + \frac{1}{M})}{W}, \quad (45)$$

which is the ratio of the two estimates, approach to unity. A typical convergence criteria is when $\hat{R} < 1.03$.

More samples.-The generation of the elements in a Markov chain is probabilistic by construction and it depends on the algorithm that we are working with. The MHA is the easiest algorithm used in bayesian inference. However there are several other algorithms that can help us to fulfill our mission. For instance, some of the most popular and effective ones apart of the MHA are the Gibbs sampling (GB) (see e.g. [? ?]), the Hamiltonian Monte Carlo (see e.g. [? ?]) or the Importance sampling (see e.g. [?]).

Autocorrelation proves.- A complementary way to look for convergence in a MCMC estimation is by looking for the autocorrelation between the samples. The *lag k* autocorrelation is defined as the correlation between every sample

and the sample k steps before. It can be quantified as [?]]

$$\rho_k = \frac{Cov(X_t, X_{t+k})}{\sqrt{Var(X_t)Var(X_{t+k})}} = \frac{E[(X_t - X)(X_{t+k} - X)]}{\sqrt{E[(X_t - X)^2]E[(X_{t+k} - X)^2]}} \quad (46)$$

where X_i is the i -th sample and X is the mean of the samples. This autocorrelation should become smaller as long as k increases (this means that samples start to become independent).

Thinning the chains.- There are several bayesian statisticians that usually thin its MCMC, it is, they do not prefer to save every step given by the MCMC; instead, they prefer to save a new step each time n steps have taken place. An obvious consequence that follows by thinning the chains is that the amount of autocorrelation is reduced. However, as long as the chains are thinned, the precision for the estimated parameters is reduced [?]. Thinning the chains can be useful in other kind of circumstances, for example, if we have limitations in memory. Notice that thinning a chain does not yield incorrect results; it yields correct results but less efficient than using the full chain.

Combining data set

Temperature of the chains

BAYESIAN STATISTIC AND COSMOLOGY

Along the new age of cosmology, observational experiments have been very helpful to confront, eliminate or refined several cosmological models. On this period it has been necessary to improve sensitivity to the experiments in order to achieve stronger constraints on the different models and model's parameters. For example, on CMB satellite experiments, there was a factor of 10 better in sensitive from *COBE* to *WMAP* and from *WMAP* to Planck [?]. On redshift surveys experiments which are interested to map the universe in redshift space, we can compare the 18,000 redshift bright galaxies that were measured by the CfA2 Redshift Survey on 1995 with the [number] of galaxies that the Sloan Digital Sky Survey (SDSS) measured on (year) [?]. In addition there are several new cosmological observations that pretend to update and make our data more precise and that we will need to confront with our models or model's parameters. Such experiments are, for example (Nuevos experimentos. Explicarlos un poco. Aquí entonces comenzar a hablar de que estos nuevos datos se pueden utilizar para constreñir parámetros).

A first example in parameter inference for Cosmology

The simplest way to understand how all these concepts can be useful in cosmology is applying them to an example. We consider the typical example in cosmology for parameter inference, which is, we estimate the value of the Hubble parameter H_0 at our present time and the density of matter in the Universe Ω_m , considering a Λ CDM cosmology. In this section we present the results of a complete work session. We wrote our own Python code using the PyMC Python's module [ref]. For interested readers, the code can be seen in appendix [B]. Notice that this can be used not only in cosmology but also in whatever model that you most prefer; what you need to do in order to prove a new model is only specify it in "pm.model()".

What is the model and the theory?

The standard Λ CDM cosmology considers a flat Universe which contains around $\sim 31\%$ of ordinary matter plus dark matter and $\sim 68\%$ of dark energy. In this Λ CDM model it is consider that the matter component of the universe follows an equation of state given by $p = 0$, while the dark energy is a cosmological constant, i.e. $p = -\rho$. In this way, considering this components, the Universe's dynamics would be given by the Friedmann equation

$$H^2 \equiv \left(\frac{\dot{a}}{a}\right) = H_0^2[\Omega_m(1+z)^3 + \Omega_\Lambda] \quad (47)$$

and the acceleration equation³. Here H is the Hubble parameter, H_0 corresponds with the Hubble parameter at present, Ω_m and Ω_Λ is the matter and dark energy densities at our epoch and follows the constraining condition $\Omega_m + \Omega_\Lambda = 1$, and z is the redshift which is associated with a time parameter; $z = 0$ is at present. Notice that thanks to the constraining condition we can rewrite $\Omega_\Lambda = 1 - \Omega_m$ and then we can reduce by one the number of parameters in the model.

The observables and the data

It is possible to measure $H(z)$ by using what it is known as the *cosmic chronometer* approach [?]. We use the data reported in [?] as our data for our estimation. A plot of them can be seen in figure ??.

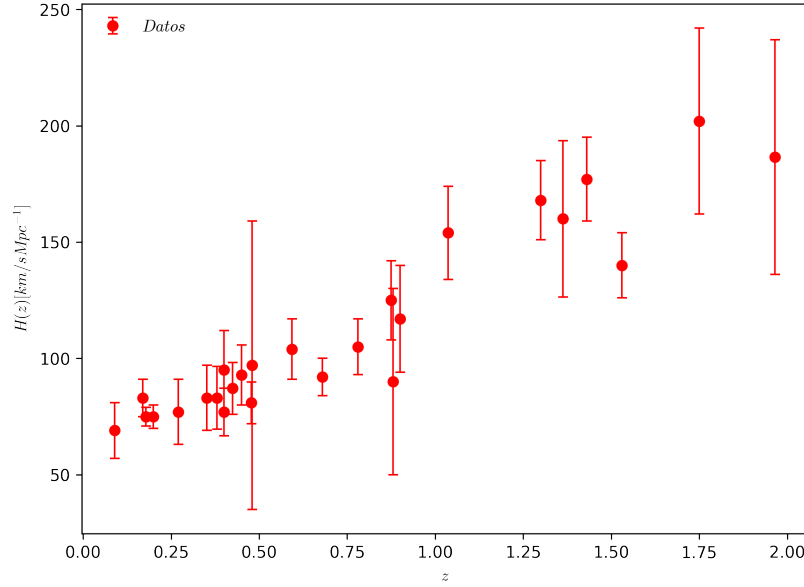


FIG. 7: Multiple MCMC. We calculate 5 Markov chains to estimate convergence of our chains.

Inferring the free parameters of the model

Now, giving a model and a set of data, we are ready to apply what we have learned until now. First of all, notice that the only free parameters in our model are Ω_m (or Ω_Λ) and H_0 . We suppose that we don't know anything about our free parameters, in such case a good prior for them is a Uniform distribution. However, in order to simplify our life we consider that we know something about the limit values for both parameters, say: $\Omega_m \in [0.1, 1]$ and $H_0 \in [10, 100]$. In this way we have as our priors

$$\Omega_m \sim U[0.1, 1] \quad (48a)$$

$$H_0 \sim U[10, 100] \quad (48b)$$

What is next?

Una vez de que ya entedimos los procedimientos para la inferencia de parámetros, hablar de que el siguiente paso es saber que hay varios códigos que ya hacen todo lo que vimos (tanto la cosmología, como la estadística) y que es mejor aprender a moverles que andar haciendo nuestro propio cdigo (quizás)

³ We do not show this equation because it is not necessary for our estimation and we do not want to confuse the reader.

Statistical codes

Once our cosmological model is established we need a statistical code which can help us to estimate the free parameters of our model. A first idea could be continuing programming our own MCMC code, but, as it is expected, while the number of free parameters of our model increases, it is more challenging to construct an efficient code. Fortunately there are several MCMC codes free to download on-line that can make this homework taking as our theory the cosmological codes showed above. In this section we review the most common of them.

Monte Python.- Monte Python is a Monte Carlo code for Cosmological Parameter extraction that can be downloaded in [?]. It contains likelihood codes of most recent experiments, and interfaces with the Boltzmann code Class for computing the cosmological observables.

The code contains several sampling methods available: Metropolis-Hastings, Nested Sampling (through MultiNest), EMCEE (through CosmoHammer) and Importance Sampling. If you are interested to work with this parameter inference code you can get help in [?] and [?].

CosmoMC.- CosmoMC (to download [?]) is a fortran 2003 MCMC engine for exploring cosmological parameter space. It contains Monte Carlo samples and importance sampling. It contains likelihoods of most recent experiments, and interfaces with CAMB.

SimpleMC.- SimpleMC is a MCMC code for cosmological parameter estimation where only expansion history matters. It was written by Ane Slosar and Jose Vazquez and can be downloaded on [?]

Some examples

Examples of cosmology

Conclusions

A. A simple MCMC python code

Here we show our MCMC written in Python. This code is very simple and its propose is to help the reader to understand how to programming a MCMC code. However, if you are interested in more sophisticated algorithms you can see the PyMC module of python [ref]. We wrote our code using the jupyter notebook [ref] which is a excellent editor when we have a program no much extense.

```
'''The necessary packages for our MCMC code'''
```

```
import matplotlib.pyplot as plt
import numpy as np
import scipy.stats as st
```

```
'''Calculate the posterior'''
```

```
def target(lik, prior, param, theta):
    if theta < 0 or theta > 1:
        return 0
    else:
        return lik(param[0], theta).pmf(param[1])*prior.pdf(theta)
```

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[1] The Shapley - Curtis Debate in 1920, [https : //apod.nasa.gov/diamond_jubilee/debate_1920.html](https://apod.nasa.gov/diamond_jubilee/debate_1920.html), visited on December 2017

```

param = 14,10 #our initial data: 14 tries and 10 heads
a = 1 #Params for the beta function
b = 1

lik = st.binom #Our likelihood
prior = st.beta(a,b) #Our prior
sigma = 0.01 #Standar desviation for the gaussian proposal distribution

naccept = 0. #Accepted steps
theta = 0.1 #Our guest for p

nitters = 100000 #How many iterations we want to do
samples = np.zeros(nitters+1)
samples[0] = theta

for i in range(nitters):
    theta_p = theta + st.norm(0, sigma).rvs()
    rho = min(1, target(lik, prior, param, theta_p)/target(lik, prior, param, theta))
    u = np.random.uniform()
    '''Metropolis Hasting algorithm'''
    if u < rho:
        naccept += 1
        theta = theta_p
    samples[i+1] = theta
nmcnc = len(samples)//2
print ("Efficiency = ", naccept/nitters)

```

```

'''We can plot our posterior results'''
thetas = np.linspace(0, 1, 200)
post = st.beta(param[1]+a, param[0]-param[1]+b)
ci = post.interval(0.95) #Our confidence interval

plt.style.use('ggplot') #It is only for the style of the plot
plt.figure(figsize=(12, 9))
plt.hist(samples[nmcnc:], 40, histtype='step', normed=True, linewidth=1, label='Distribution of posterior samples')
plt.hist(prior.rvs(nmcnc), 40, histtype='step', normed=True, linewidth=1, label='Distribution of prior samples');
plt.plot(thetas, post.pdf(thetas), c='red', linestyle='--', alpha=0.5, label='True posterior')
plt.axhline(0.3, ci[0], ci[1], c='black', linewidth=2, label='95% CI');
plt.xlim([0,1]);
plt.legend(loc='best');
plt.show()

```

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